

A complexity measure for continuous time quantum algorithms

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We consider unitary dynamical evolutions on n qubits caused by time dependent pair-interaction Hamiltonians and show that the running time of a parallelized two-qubit gate network simulating the evolution is given by the time integral over the chromatic index of the interaction graph. This defines a complexity measure of continuous and discrete quantum algorithms which are in exact one-to-one correspondence. Furthermore we prove a lower bound on the growth of large-scale entanglement depending on the chromatic index.

I. INTRODUCTION

At the moment, the most popular model of a quantum computer consists of the 2^n dimensional Hilbert space $\mathcal{H}_n := (\mathbb{C}^2)^{\otimes n}$ of ‘ n qubits’ as its memory space, and some one- and two-qubit gates as its set of basic transformations (see e.g. [1]). There are several reasons for taking one- and two-qubit gates as the basic ones: Firstly, from the pure mathematical point of view, it is quite natural to look for a subset of the Lie group of unitary transformations on the Hilbert space \mathcal{H}_n generating the whole group. Obviously, one-qubit operations do not generate the whole Lie group, the set of two-qubit gates does [2]. Hence there is no reason for taking more complicated transformations like three-qubit unitary operators as basic ones. Secondly, the model of two-qubit gates might be considered as the attempt to develop quantum computation in strong analogy to the theory of classical devices: Building complex logical networks from two-bit gates is a successful concept of classical computation. The third reason stems from physics. Unfortunately it is only ‘a little bit’ convincing: From the fundamental point of view, n particles interact always in the form of pair-interactions, i.e., the total Hamiltonian H of the system can be decomposed as

$$H = \sum_{k,l \leq n} H_{k,l} + \sum_{j \leq n} H_j$$

where $H_{k,l}$ is a self-adjoint operator acting on the joint Hilbert space of particle k and l and H_j is the free Hamiltonian of particle j (without loss of generality, we can drop the second sum, by reckoning it to the first part). Pair-interactions $H_{k,l}$ are the infinitesimal versions of two-qubit gates: every unitary of the form $e^{iH_{k,l}t}$ for $t \in \mathbb{R}$ is a two-qubit gate. On the one hand, this seems to be an important justification for two-qubit gates, since it refers to the form of the fundamental forces of nature, on the other hand, the argument is not really correct: In general there is no obvious correspondence between the time evolution

$$e^{i \sum H_{k,l} t} \quad (1)$$

and any finite sequence of two-qubit gates. However, there is an obvious simulation by two-qubit gates in an *approximative* sense given by the well-known Trotter formula:

$$\lim_{m \rightarrow \infty} (\prod_{k,l} e^{iH_{k,l}t/m})^m = e^{i \sum_{k,l} H_{k,l}t}. \quad (2)$$

This example shows, that the simulation of the time evolution caused by a time-independent pair-interaction Hamiltonian might require an *infinite* number of two qubit gates. Hence it seems to suggest that a definition of complexity based on two-qubit gates does *not* take into account the most natural form of dynamics of many-particle quantum physics. However, it has been shown [3] that the number m of gates required to simulate the right hand side of (2) up to an error ϵ is only growing with t^2/ϵ . Despite the fact that infinite accuracy requires an infinite number of gates, the *time* for implementing the growing number of unitaries does not tend to infinity if one assumes that the implementation of $e^{iH_{k,l}t/m}$ requires the time $O(t/m)$ (see [3]). Taking this assumption, we will show that the running time of a discrete quantum algorithm for simulating the dynamics given by (1) is determined by the chromatic index of the interaction graph. This turns out to be true even for time-dependent pair-interactions. One might reformulate this result by saying that the running time depends on ‘the complexity of the interaction’. The relevance of this result is twofold: In case realizations of future quantum computers are based on two-qubit gates, it gives exact statements about the complexity of simulating non-autonomous quantum dynamics resulting from pair-interaction Hamiltonians. To our knowledge, this is the first exact analogue between complexity measures of discrete and continuous quantum algorithms. Secondly, our result is relevant for the simulation of arbitrary pair-interaction dynamics by a dynamic with restricted interaction graph: We derive statements about the efficiency for simulating time evolutions based on pair-interactions with *high chromatic index* by other evolutions with interactions of *lower index*.

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II. DISCRETE AND CONTINUOUS QUANTUM ALGORITHMS

In our model of discrete quantum computers, two-qubit gates acting on disjoint pairs of qubits can be implemented simultaneously. We define:

Definition 1 A discrete quantum algorithm A of depth k is a sequence of k steps $\{A_1, \dots, A_k\}$ where every step consists of a set of two qubit gates $\{u_{jl}\}_{j,l}$ acting on disjoint pairs (j,l) of qubits. Every step i defines a unitary operator v_i by taking the product of all corresponding unitaries in any order. The product $u := \prod_{i \leq k} v_i$ is the ‘unitary operator implemented by A ’.

The following quantity measures the deviation of a unitary operator from the identity:

Definition 2 The angle of an arbitrary unitary operator u is the smallest possible norm¹ $\|a\|$ of a selfadjoint operator a which satisfies $e^{ia} = u$. It coincides with the time required for the implementation of u if the norm of the used Hamiltonian is 1.

This term allows us to formulate a modification of the term ‘depth’ which will later turn out to be decisive in connecting complexity measures of discrete and continuous algorithms:

Definition 3 Let α_i be the maximal angle of the unitaries performed in step i . Then the **weighted depth** is defined to be the sum $\sum_i \alpha_i$.

Assuming that the implementation time of a unitary is proportional to its angle, the weighted depth is the running time of the algorithm. Since this coincidence is based on a possibly unrealistic assumption we will prefer the term ‘weighted depth’ in formulating exact mathematical statements.

Now we want to formalize the notion of quantum algorithms based on time dependent Hamiltonians. Such continuous algorithms have already been considered in the literature² (e.g. see [4–9]), but in our approach the Hamiltonians are explicitly restricted to pair-interactions in many-particle systems:

Definition 4 A continuous quantum algorithm A of running time T is a piecewise Lipschitz continuous function $t \mapsto H(t)$ from the interval $[0, T]$ into the set of those self-adjoint operators acting on \mathcal{H}_n which can be decomposed into

$$H(t) = \sum_{k,l} H_{k,l}(t),$$

where every $H_{k,l}$ is a self-adjoint operator acting on the qubits k and l . Here $H_{k,l} = H_{l,k}$ and the sum runs over the unordered pairs. We say ‘ A implements u ’ if $u = u_T$ and $(u_t)_{t \in T}$ is the solution of the non-autonomous differential equation $\frac{d}{dt}u_t = -iH(t)$ with $u_0 = 1$.

As already mentioned above, the weighted depth of a discrete algorithm for simulating the evolution (1) is finite. More precisely, it is at most mt if m is the number of pairs (k,l) with the property that $H_{k,l} \neq 0$. But, if one has additional information about the interactions, one can make further statements about possible parallelization. This is illustrated by the following examples: In case all the pairs (k,l) with $H_{k,l} \neq 0$ are disjoint, we can perform all the unitaries $e^{iH_{k,l}t/m}$ simultaneously and get the running time t . In case of the nearest-neighbor interaction in a one dimensional spin chain, we have only pairs of the form $(k, k+1)$. Hence we can perform all the transformations

$$e^{iH_{2k,2k+1}t/m}$$

simultaneously and the operations

$$e^{iH_{2k+1,2k+2}t/m}$$

as well. Here, parallelization allows to decrease the running time down to $2t$.

We show that the graph theoretical concept of chromatic index offers the appropriate terminology for determining the degree of possible parallelization.

Definition 5 [10] The **chromatic index** of a graph with vertices $\{1, \dots, n\}$ is the least number of colors required for coloring the edges in such a way that there are no edges with the same color having a common vertex.

For every time t during the running time of the continuous algorithm we define a family of undirected graphs:

Definition 6 For every non-negative real number r and every time $t \in [0, T]$ we define the **interaction graph** $G_r(t)$ as follows: Take the qubits $\{1, \dots, n\}$ as vertices and let the edges be all the pairs (k,l) with the property $\|H_{k,l}(t)\| > r$.

The following quantity turns out to be decisive for the degree of possible parallelization of the discrete simulation:

¹Here and in the following $\|\cdot\|$ denotes the operator norm given by $\|a\| := \max_x \|ax\|$ where x runs over the unit vectors of the corresponding Hilbert space.

²In [4] time-dependent Hamiltonian algorithms are called an ‘analog analogue of a digital quantum computer’.

Definition 7 Let $n_r(t)$ be the chromatic index of $G_r(t)$. For any time $t \in [0, T]$ of a continuous algorithm we define the **weighted chromatic index** $W(t)$ as

$$W(t) := \int_0^\infty n_r(t) dr.$$

Furthermore we will need the time integral of W :

Definition 8 The **integrated chromatic index** of the quantum algorithm is defined to be

$$I := \int_0^T \int_0^\infty n_r(t) dr dt,$$

where T is the running time of the continuous algorithm.

Actually, the terminology ‘integrated weighted chromatic index’ would be appropriate. We preferred the short terminology.

III. TRANSLATION BETWEEN DISCRETE AND CONTINUOUS ALGORITHMS

The following theorem suggests that the simulation of an interaction with high integrated chromatic index generically requires a discrete algorithm with high weighted depth. More precisely, it shows that the complexity of a unitary transformation can equivalently be defined as the infimum over the values of the weighted depth of all possible discrete implementations or the infimum over the values of the integrated chromatic index of all possible continuous implementations:

Theorem 1

a) Every arbitrary unitary operator u acting on n qubits which can be implemented by a discrete quantum algorithm with weighted depth α can also be implemented by a continuous quantum algorithm with integrated chromatic index α .

b) If there is a continuous algorithm with integrated chromatic index α implementing u then there is a sequence of discrete algorithms $(A_k)_{k \in \mathbb{N}}$ implementing the unitaries u_k such that $\lim_{k \rightarrow \infty} u_k = u$ and the corresponding values of the weighted depth converge to α .

Proof: Statement a) is almost trivial: Let A be a discrete quantum algorithm of depth k with the maximal angles $(\alpha_j)_{j \leq k}$. Let \mathcal{S}_j be the set of qubit pairs which are addressed in the step j and $(u_p)_{p \in \mathcal{S}_j}$ the corresponding set of unitary transformations. Define a continuous algorithm with running time k as follows: for $t \in (j-1, j)$ we³ define the constant Hamiltonian $H(t) := \sum_{p \in \mathcal{S}_j} -i \ln u_p$.

Since the angle of a unitary operator u is the norm of $\ln u$, we have $\alpha_j = \max_{p \in \mathcal{S}_j} \|\ln u_p\|$. Hence, for every t in the interval $(j-1, j)$ we have $n_r(t) = 0$ for $r \geq \alpha_j$ and $n_r(t) = 1$ otherwise. Obviously we have

$$\int_0^T \int_0^\infty n_r(t) dr dt = \sum_j \alpha_j.$$

For statement b) take a partition of $[0, T]$ into small intervals on which H is continuous. Let $(t, t + \epsilon)$ be one of those intervals. Let

$$r_1 < \dots < r_m$$

be the positive numbers $(\|H_{i,j}(t + \epsilon/2)\|)_{i,j \leq n}$ in its canonical ordering. Furthermore define $r_0 := 0$. Obviously, the function $r \mapsto n_r(t + \epsilon/2)$ takes constant values n_j on every interval $[r_{j-1}, r_j]$ for $1 \leq j \leq m$. Let

$$M_1 \cup M_2 \cup \dots \cup M_{n_j}$$

be a partition of the set of edges of $G_{r_j}(t + \epsilon/2)$ given by an allowed coloring (in the sense of Definition 5) of the edges corresponding to the chromatic index n_j . For every $j \leq m$ we proceed as follows: For every M_p define a step of a discrete algorithm by the set of unitaries

$$\left\{ e^{(i\epsilon H_{k,l}(t+\epsilon/2)) \times (r_j - r_{j-1}) / \|H_{k,l}(t+\epsilon/2)\|} \right\}_{(k,l) \in M_p}.$$

Since p runs from 1 to n_j we obtain n_j steps for the discrete algorithm. Every step has at most the angle $\epsilon(r_j - r_{j-1})$. The weighted depth of these n_j steps is at most $n_j \epsilon(r_j - r_{j-1})$. Doing this for every $j \leq m$, we obtain a sequence of $\sum_{j \leq m} n_j$ steps which substitutes the continuous algorithm on the interval $(t, t + \epsilon)$ up to an error in the order of ϵ^2 . The weighted depth of this sequence is at most

$$\sum_{1 \leq j \leq m} n_j \epsilon(r_j - r_{j-1}) = \epsilon \int_0^\infty n_r(t + \epsilon/2) dr. \quad (3)$$

Without loss of generality we will assume the weighted depth to be *equal* to the terms in equation (3) since we can blow up the algorithm by transformations which cancel each other out. If the total discrete algorithm is defined by combining the sequences for every interval of the form $(s, s + \epsilon)$ we get a simulation of the continuous algorithm with an error in the order of ϵ . Furthermore the total weighted depth converges to $\int_0^T \int_0^\infty n_r(t) dt$ for $\epsilon \rightarrow 0$. \square

One can consider discrete quantum algorithms as special cases of continuous quantum algorithms in the sense

³Here we denote an interval by $(.)$ if we do not care about whether it is open or closed.

of the proof of part a) of Theorem 1. Then the discrete quantum computer is obtained by restricting the Hamiltonians $H(t)$ to those with chromatic index one and norm one for each non-vanishing component $H_{k,l}(t)$. In this sense, part a) of Theorem 1 is a special case of the general principle that continuous time algorithms can be simulated by other continuous time algorithms with lower chromatic indices and the same strength of the pair-interactions where the running time is increased by the quotient of the chromatic indices. We sketch this simple observation in a not too formal way:

At time t we have the interaction

$$H(t) := \sum_{(j,l)} H_{j,l}(t),$$

where (j,l) runs over the edges E of the graph $G_0(t)$. For $m < n_0(t)$ take k such that $km \geq n_0(t)$. Take a partition of the edges of $G_0(t)$ into k subsets such that the subgraphs with the set of edges $(E_i)_{i \leq k}$ have chromatic indices less or equal to m . Substitute the small time interval $(t, t + \epsilon)$ of the original algorithm by the k time intervals $(t + (i-1)\epsilon, t + i\epsilon)$ with $1 \leq i \leq k$ in which the Hamiltonian $\sum_{(j,l) \in E_i} H_{j,l}(t + \epsilon/2)$ is switched on. The difference of the unitary operators implemented by the substituted algorithm and the original one is of second order in ϵ for every subinterval. Hence the total error tends to zero for $\epsilon \rightarrow 0$.

This observation justifies in some sense our point of view that one might think of the chromatic index as the complexity of the interaction. This raises the question whether bounds can be given on the required integrated chromatic index necessary for preparing certain entangled quantum states from an initial product state.

IV. COMPLEXITY BOUNDS FOR HIGH ENTANGLEMENT

In [11] we gave lower bounds on the depth required for preparing certain states with large-scale entanglement (some of those bounds are easy conclusions from [12]) for large qubit numbers n . More specifically, one can show the following: Let $(a_j)_{j \leq n}$ be a family of arbitrary self-adjoint operators where every a_j acts on qubit j and has operator norm 1. For product states, the variance of the observable

$$a := \sum_{j \leq n} a_j \quad (4)$$

grows with $O(n)$. Values of the variance in the order of n^2 indicate large-scale entanglement for pure states [13]. In a state obtained by a discrete algorithm with depth k we could show [11] the variance to be less or equal to $n 4^k/2$. Hence the emergence of large-scale entanglement in the sense described above requires a depth in the order of $\log n$.

It is natural to ask whether similar bounds can be shown for the *weighted* depth and the integrated chromatic index. However, below we present a proof for such a bound. In contrast to the discrete definition of depth the bound is asymptotically independent on n in the limit $n \rightarrow \infty$. Whether this is a lack of our estimations or whether it is a hint for a fundamental difference between complexity measures of continuous and discrete algorithms is unclear. We have:

Theorem 2 *Let $t \mapsto H(t)$ be a continuous quantum algorithm with integrated chromatic index α implementing the unitary u . Let the quantum computer start in the product state $\rho^{\otimes n}$. Let $\sigma := u(\rho^{\otimes n})u^\dagger$ be the state obtained by the algorithm. Then for the variance of any observable a of the form (4) in the state σ we have*

$$V_\sigma(a) \leq \frac{n}{(1-2\alpha)^4}$$

with

$$\begin{aligned} V_\sigma(a) &:= \text{tr}(\sigma a^2) - (\text{tr}(\sigma a))^2 \\ &= \text{tr}(\rho^{\otimes n} (u^\dagger a u)(u^\dagger a u)) - \text{tr}(\rho^{\otimes n} (u^\dagger a u))^2. \end{aligned}$$

Proof: Due to Theorem 1 we can restrict the proof to the case that H is of the same form as that one constructed in the proof of Theorem 1 a), i.e., $H(t)$ is for every t a sum of pair-interactions acting on disjoint pairs. Furthermore we will assume without loss of generality that the norm of every non-vanishing pair-interaction is one. Then α coincides with the running time T . We write $H(t) = \sum_{e \in E(t)} H_e(t)$ where $E(t)$ is the set of edges of the interaction graph $G_0(t)$. By solving the differential equation

$$\frac{d}{dt} a(t) = i[H(t), a(t)]$$

with $a(0) = a$ we obtain $u^\dagger a u = a(T)$. Explicitly, $u^\dagger a u$ is given by a Dyson series [14]:

$$u^\dagger a u = \sum_{k \in \mathbb{N}} i^k \int [H(t_k), [\dots, [H(t_1), a] \dots]] dt^k,$$

where the integration is carried out over the simplex

$$0 \leq t_1 \leq \dots \leq t_k \leq T.$$

Let $X := (p_k, \dots, p_1, r)$ be a $k+1$ tuple consisting of k unordered pairs p_j (which are considered as subsets of $\{1, \dots, n\}$) and one element $r \in \{1, \dots, n\}$. Define

$$\begin{aligned} B_X(t_k, \dots, t_1) &:= \\ &[H_{p_k}(t_k), [H_{p_{k-1}}(t_{k-1}), [\dots, [H_{p_1}(t_1), a_r] \dots]]]. \end{aligned}$$

Furthermore, for an arbitrary pair of observables c, d we introduce the covariance $C(c, d)$ in the state $\rho^{\otimes n}$ as

$$C(c, d) := \text{tr}(\rho^{\otimes n} c d) - \text{tr}(\rho^{\otimes n} c) \text{tr}(\rho^{\otimes n} d).$$

Then the variance of the observable a in the state σ can be written as:

$$V_\sigma(a) = \sum_{k,l} F_{k,l}$$

with

$$F_{k,l} := \int \int \sum_{X,Y} C(B_X(t_k, \dots, t_1) B_Y(s_l, \dots, s_1)) dt^k ds^l,$$

where the sum runs over all $(k+1)$ -tuples X of the form $X := (e_k, \dots, e_1, r)$ with $e_j \in E(t_j) \forall j$ and $r \in \{1, \dots, n\}$ and $(l+1)$ -tuples Y which are defined analogously by using the sets of edges $E(s_j)$ instead of $E(t_j)$ (here k runs over all non-negative integers). In the following, we shall sometimes consider an X of this form canonically as a subset of $\{1, \dots, n\}$ and write $j \in X$ iff j agrees with the rightmost element of X or with one of the vertices of at least one e_i for $1 \leq i \leq k$.

Now let the times t_k, \dots, t_1 and s_l, \dots, s_1 be fixed. We define \mathcal{X}_k as the set of $(k+1)$ -tuples (e_k, \dots, e_1, r) with $e_j \in E(t_j)$ and the property that every e_j has a vertex which is an element of (e_{j-1}, \dots, e_1, r) . It is easy to see that $B_X(t_k, \dots, t_1) \neq 0$ implies $X \in \mathcal{X}_k$. The set \mathcal{X}_k can be constructed iteratively: Set $\mathcal{X}_0 := \{(1), \dots, (n)\}$. Then we have $(e_k, X) \in \mathcal{X}_k$ if and only if $X \in \mathcal{X}_{k-1}$ and $e_k \in E(t_k)$ and at least one of the vertices of e_k is an element of X (here (e_k, X) is an informal notation for the $(k+1)$ -tuple obtained by appending e_k to the k -tuple X). In an analogous way we define the set \mathcal{Y}_l by referring to the sets $E(s_j)$ instead of $E(t_j)$.

The covariance

$$C(B_X(t_k, \dots, t_1) B_Y(s_l, \dots, s_1)) \quad (5)$$

can only be nonzero if $X \in \mathcal{X}_k$ and $Y \in \mathcal{Y}_l$ have nonempty intersection (considered as subsets of $\{1, \dots, n\}$). We show that there are at most $n(k+1)!(l+1)!$ pairs X, Y with this property by proving that for every $j \in \{1, \dots, n\}$ there are at most $(k+1)!$ sets $X \in \mathcal{X}_k$ with $j \in X$. This can be seen by induction over k : For $k=0$ the statement is obvious. Assume the statement to be true for \mathcal{X}_{k-1} . For every $X \in \mathcal{X}_{k-1}$ with $j \in X$ we have at most $k+1$ elements of the form $(e_k, X) \in \mathcal{X}_k$ since for each vertex $v \in X$ there can be at most one $e_k \in E(t_k)$ such that e_k has v as a vertex (remember that the corresponding graph $G_0(t_k)$ has chromatic index 1). If $j \notin X$ the statement $j \in (e_k, X)$ can only be true if $j \in e_k \in E(t_k)$. There is at most one $e_k \in E(t_k)$ with vertex j . Let e_k be the pair $\{j, m\}$. By assumption there are at most $k!$ tuples $X \in \mathcal{X}_{k-1}$ such that $m \in X$. Hence there are at most $(k+1)k!$ sets $(e_k, X) \in \mathcal{X}_k$ with $j \in (e_k, X)$.

Since the norm of every $H_e(t)$ is zero or one by assumption, the norm of $B_X(t_k, \dots, t_1)$ can never exceed 2^k .

Hence we get

$$\begin{aligned} & \sum_{X \in \mathcal{X}_k, Y \in \mathcal{Y}_l} C(B_X(t_k, \dots, t_1), B_Y(s_l, \dots, s_1)) \\ & \leq n 2^k 2^l (k+1)! (l+1)!. \end{aligned}$$

Since the integration is carried out over a simplex of size $T^k T^l / (k! l!)$ we obtain:

$$\begin{aligned} V_\sigma(a) & \leq n \sum_{k,l} (2T)^k (k+1) (2T)^l (l+1) \\ & = n \left(\sum_k (2T)^k (k+1) \right)^2. \end{aligned}$$

This power series converges for $2T < 1$. Since

$$\sum_{k \in \mathbb{N}} (k+1) p^k = 1/(1-p)^2 \text{ for every } -1 < p < 1$$

we have:

$$V_\sigma(a) \leq \frac{n}{(1-2T)^4}.$$

□

Theorem 2 shows that for huge n the variance of the measurement results of any mean-field observable can only grow in the order of n^2 if the integrated chromatic index α is at least $1/2$. Hence $\alpha \geq 1/2$ is a necessary condition for the particular class of large-scale entangled states considered in [13].

V. CONCLUSIONS

We have shown that the running time of a discrete algorithm simulating the evolution defined by a time-dependent Schrödinger-equation with pair-interaction Hamiltonians is given by the time integral over the chromatic index of the interaction graph. This result suggests to take this time integral as a complexity measure for continuous time algorithms and it seems natural to ask for the complexity for the preparation of highly entangled states in many-particle systems. We proved such a bound. At the moment, we cannot decide whether it is tight or not. Given a quantum system with the property that the weighted chromatic index $W(t)$ of the relevant interaction Hamiltonian satisfies $W(t) \leq m$ for every time t we conclude that the system requires at least the time $1/(2m)$ in order to produce large-scale entanglement in the sense explained above. If we assume a non-vanishing probability of depolarizing errors for each single qubit, the error probability has to decrease with $O(1/n)$ if large-scale entanglement should be maintained [13]. This strongly suggests that the chromatic index or the strength of the interaction has to increase in the order of n .

For nearest-neighbor interactions in solid state physics it is not useful to apply our estimations, since there are

considerably tighter bounds (see [15] paragraph 6.2.1) But for mean-field interactions [16], where the weighted chromatic index $W(t)$ is already determined by the strength of the pair-interactions, we cannot see any ob-

vious tighter bounds. Hence physical systems like solid states with long-range interactions will present a typical application of our results.

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